L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2008:1459108 CAPLUS Full-text

DN 149:576645

TI Preparation of tricyclic compounds such as pyrrolobenzoxazepine derivatives and analogs thereof for treatment of hypercholesteremia, hyperlipemia, and arteriosclerosis

IN Sugita, Kazuyuki; Otsuka, Masaki; Oki, Hitoshi; Haginoya, Noriyasu; Ichikawa, Masanori; Ito, Masao

PA Daiichi Sankyo Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 1516pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 2008291018	A	20081204	JP 2008-114684	20080424		
PRAI	JP 2007-115119	A	20070425				
OS	MARPAT 149:576645						
GI							

$$\begin{array}{c|c}
R2 & R1 \\
\hline
(N) & X \\
R2? & N \\
\hline
R3 & I
\end{array}$$

AB The title compds. [I; R1 = aryl or heteroaryl which may have 1 to 3 substituents; R2, R2a = H, halo, cyano, etc.; R3 = H, halo, alkyl, etc.; R4 = carboxyl, carboxycarbonyl, carboxyalkenyl, etc.; X = CH2, O, S; Y = N, CR3a; R3a = same as defined for R3; Z = N, CR3aa; R3aa = same as defined for R3; ring (N) = benzene or pyridine ring] are prepared I inhibit squalene synthetase and cholesterol synthesis. Thus, 2-(2-(2-[(4R,6S)-8-chloro-6-(2,3-dimethoxyphenyl)-10-fluoro-4H,6H- pyrrolo[1,2-a][4,1]benzoxazepin-4-yl]ethyl)-2H-1,2,3,4-tetrazol-5- yl)acetic acid was prepared in a multistep process starting from 2-bromo-4-chloro-6-fluoroaniline and 2,5-dimethoxytetrahydrofuran. Compds. of this invention showed IC50 values of 0.56 nM to 7.6 nM against rat squalene synthetase.

IT 937062-99-2P 937064-08-9P 937064-14-7P 937064-19-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic compds. such as pyrrolobenzoxazepine derivs. and analogs thereof for treatment of hypercholesteremia, hyperlipemia, and arteriosclerosis)

RN 937062-99-2 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

RN 937064-08-9 CAPLUS

CN 5-Oxazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937064-14-7 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

RN 937064-19-2 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl-, ethyl ester, rel- (CA INDEX NAME)

```
2008:352510 CAPLUS Full-text
DN
     148:347355
     Preventive or therapeutic agent for respiratory disease
ΤI
     Matsumoto, Tatsumi
IN
     Takeda Pharmaceutical Company Limited, Japan
PA
SO
     PCT Int. Appl., 93pp.
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                            APPLICATION NO.
                                _____
     WO 2008032696
                                20080320
                                         WO 2007-JP67634
PΤ
                        A1
                                                                   20070911
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA,
             CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI,
             GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
             KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
             MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
             PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
             GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
                               20060912
PRAI JP 2006-247082
                        Α
    MARPAT 148:347355
OS
GΙ
        R3
```

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

$$\begin{array}{c}
R_2 \\
R_1
\end{array}$$

L5

ΑN

AΒ An agent for suppressing both progression and acute exacerbation of decreased respiratory function with age in respiratory disease, comprising a compound having a squalene synthase inhibitory action and represented by the formula: (I) (wherein R1 represents a hydrogen atom or a hydrocarbon group which may be substituted; R2 and R3 are the same or different and represent a hydrogen atom, a hydrocarbon group which may be substituted or the like; X' represents a carboxyl group which may be esterified, a carbamoyl group which may be substituted, a hydroxy group which may be substituted, an amino group which may be substituted, or a group constituted by a heterocyclic residue which has a deprotonatable hydrogen atom and may be substituted; the ring A represents a benzene ring or a heterocyclic ring which may be substituted; the ring J' represents a 7- or 8-membered heterocyclic ring containing 3 or less heteroatoms as ring constituent atoms, and the ring J' may further have a substituent other than R1, R2, R3 and X').

839724-36-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(benzoxacepinylpiperidine analogs and prodrugs as squalene synthase inhibitors and preventive or therapeutic agents for respiratory disease)

839724-36-6 CAPLUS RN

1,2,4-Oxadiazole-5-pentanoic acid, CN

3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-

1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME) Absolute stereochemistry.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
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AN 2007:538026 CAPLUS Full-text

DN 147:9956

TI Preparation of tricyclic compounds such as pyrrolobenzoxazepine derivatives and analogs thereof for treatment of hypercholesteremia, hyperlipemia, and arteriosclerosis

IN Sugita, Kazuyuki; Otsuka, Masami; Oki, Hitoshi; Haginoya, Noriyasu; Ichikawa, Masanori; Itoh, Masao

PA Daiichi Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 1709pp. CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

11111	PATENT NO.				KIND DATE			APPLICATION NO.										
ΡI	WO 2007055093		A1 20070518		WO 2006-JP321056													
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
			GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚM,	KN,
			KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,
			MN,	MW,	MX,	MY,	MΖ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,
			RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ΤJ,	TM,	TN,	TR,	TT,
			TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW						
		RW:	ΑT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
			IS,	ΙT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	BJ,
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
			GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
			KG,	KΖ,	MD,	RU,	ТJ,	TM										
	ΕP	EP 1939205		A1	20080702			EP 2006-832385						20061023				
		R:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
			IS,	ΙT,	LI,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,
			BA,	HR,	MK,	RS												
PRAI	JP	JP 2005-306663			Α		2005	1021										
	WO 2006-JP321056			6	W		2006	1023										
OS GI	MARPAT 147:9956																	

$$\begin{array}{c|c}
R^2 & R^1 \\
\hline
(N) & X \\
R^2 & X
\end{array}$$

$$\begin{array}{c|c}
R^4 & X \\
R^4 & X \\
\end{array}$$

The title compds. I [R1 = aryl or heteroaryl which may have 1 to 3 substituents; R2, R2a = H, halo, cyano, etc.; R3 = H, halo, alkyl, etc.; R4 = carboxyl, carboxycarbonyl, carboxyalkenyl, etc.; X = CH2, O, S; Y = N, CR3a; R3a = same as defined for R3; Z = N, CR3aa; R3aa = same as defined for R3; ring (N) = benzene or pyridine ring] are prepared I inhibit squalene synthetase and cholesterol synthesis. Thus, 2-(2-(2-[(4R,6S)-8-chloro-6-(2,3-dimethoxyphenyl)-10-fluoro-4H,6H- pyrrolo[1,2-a][4,1]benzoxazepin-4-yl]ethyl)-2H-1,2,3,4-tetrazol-5- yl)acetic acid was prepared in a multistep process

starting from 2-bromo-4-chloro-6-fluoroaniline and 2,5-

dimethoxytetrahydrofuran. Compds. of this invention showed IC50 values of $0.56\,$ nM to $7.6\,$ nM against rat squalene synthetase.

IT 937062-99-2P 937064-08-9P 937064-14-7P

937064-19-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic compds. such as pyrrolobenzoxazepine derivs. and analogs thereof for treatment of hypercholesteremia, hyperlipemia, and arteriosclerosis)

RN 937062-99-2 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937064-08-9 CAPLUS

CN 5-Oxazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

RN 937064-14-7 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]methyl]-, methyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 937064-19-2 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]methyl]-4-methyl-, ethyl ester, rel- (CA INDEX NAME)

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2006:1224848 CAPLUS Full-text

DN 146:134491

TI Chemical Database Mining through Entropy-Based Molecular Similarity Assessment of Randomly Generated Structural Fragment Populations

AU Batista, Jose; Bajorath, Juergen

CS Department of Life Science Informatics, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany

SO Journal of Chemical Information and Modeling (2007), 47(1), 59-68 CODEN: JCISD8; ISSN: 1549-9596

PB American Chemical Society

DT Journal

LA English

The authors describe a novel approach to search for active compds. that is AΒ based on the generation of random mol. fragment populations. As a similaritybased methodol., fragment profiling does not depend on the use of predefined descriptors of mol. structure and properties and the design of chemical space representations. To adapt the generation and comparison of random fragment populations for large-scale compound screening, the authors compare different fragmentation schemes, introduce the concept of compound class-specific fragment frequencies, and develop a novel entropic similarity metric for compound ranking. The approach has been extensively tested on 15 different compound activity classes with varying degrees of intraclass structural diversity and produced promising results in these calcns., comparable to similarity searching using fingerprints. A key feature of fragment profile searching is that the calcn. of compound class-specific proportional Shannon entropy of random fragment distributions enables the identification of database mols. that share a significant number of signature substructures with known active compds.

IT 606928-75-0

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(chemical database mining through entropy-based mol. similarity assessment)

RN 606928-75-0 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-3-[2-(3,4-dihydro-1(2H)-pyridinyl)-2-oxoethyl]-5-(2,3-dimethoxyphenyl)-1,5-dihydro-, (3R,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L5
    ANSWER 5 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ΑN
    2006:1147695 CAPLUS Full-text
DN
    145:465761
    Remedy for xanthoma containing squalene synthetase inhibitor
ΤI
    Shiomi, Masashi; Ito, Takashi; Tozawa, Ryuichi; Amano, Yuichiro
IN
    National University Corporation Kobe University, Japan; Takeda
PA
    Pharmaceutical Company Limited
    PCT Int. Appl., 102pp.
SO
    CODEN: PIXXD2
DT
    Patent
    Japanese
LA
FAN.CNT 1
    PATENT NO.
                      KIND
                              DATE
                                     APPLICATION NO. DATE
                             _____
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                                          _____
                              20061102 WO 2006-JP308402
    WO 2006115193
РΤ
                        A1
                                                                20060421
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
            KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
            MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
            SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
            VN, YU, ZA, ZM, ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
            IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
            CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
            GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM
                               20061102
    AU 2006240710
                       A1
                                          AU 2006-240710
                                                                 20060421
    CA 2605365
                               20061102
                                          CA 2006-2605365
                        Α1
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    EP 1889632
                        Α1
                               20080220
                                          EP 2006-745533
                                                                 20060421
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            BA, HR, MK, YU
                                          IN 2007-KN3945
    IN 2007KN03945
                        Α
                               20080125
                                                                 20071015
    MX 2007012935
                        Α
                               20080326
                                          MX 2007-12935
                                                                 20071017
                                         KR 2007-724160
    KR 2008015395
                       A
                             20080219
                                                                 20071019
    NO 2007005387
                                         NO 2007-5387
                        Α
                             20080121
                                                                 20071022
    CN 101203243
                                         CN 2006-80022653 20071224
                        Α
                             20080618
PRAI JP 2005-124781
                              20050422
                        Α
    WO 2006-JP308402
                        W
                              20060421
                       W
    WO 2006-JP8402
                             20060421
OS
    MARPAT 145:465761
AB
    Disclosed is a preventive/remedy for xanthoma which contains a compound having
     an inhibitory effect on squalene synthase, its prodrug or its salt. For
     example, the effect of N-[(3R,5S)-1-(3-acetoxy-2,2-dimethylpropyl)-7-chloro-
     5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepine-3-
     acetyl]piperidine-4-acetic acid (I) on xanthoma in rabbits was examined Also,
     a capsule containing I 10 mg/capsule was formulated.
ΙT
    839723-32-9 839723-37-4 839723-87-4
    839724-23-1 839724-36-6 839725-28-9
    839725-30-3 913621-84-8
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (remedies for xanthoma containing squalene synthetase inhibitors)
RN
    839723-32-9 CAPLUS
    5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-
CN
    1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-
    3-y1]methy1]- (CA INDEX NAME)
```

RN 839723-37-4 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-87-4 CAPLUS

CN Benzeneacetic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

RN 839724-23-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-36-6 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_3C$$
 ON
 R
 S
 $C1$
 MeO
 OMe

RN 839725-28-9 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839725-30-3 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(CA INDEX NAME)

Absolute stereochemistry.

RN 913621-84-8 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-(CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
DN
     142:219318
     Preparation of benzoxazepine derivatives as squalene synthase inhibitors
ΤI
     Marui, Shogo; Miki, Takashi; Miura, Shoutarou; Nishimoto, Tomoyuki;
ΙN
     Nakada, Yoshihisa
     Takeda Chemical Industries, Ltd., Japan
PA
     PCT Int. Appl., 239 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                        KIND
                               DATE
                                           APPLICATION NO.
                                                                  DATE
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     WO 2005012272
                                20050210
                                          WO 2004-JP11293
PΤ
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
                                           AU 2004-260757
     AU 2004260757
                         Α1
                               20050210
                                                                   20040730
     CA 2534464
                                           CA 2004-2534464
                         Α1
                               20050210
                                                                   20040730
     JP 2005068138
                         Α
                               20050317
                                            JP 2004-222658
                                                                   20040730
     EP 1650201
                               20060426
                                           EP 2004-748264
                         Α1
                                                                   20040730
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK,
     CN 1832934
                         Α
                               20060913
                                           CN 2004-80022202
                                                                   20040730
     BR 2004013009
                         Α
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     WO 2004-JP11293
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AΒ The title compds. I (ring A and ring B each represents an optionally substituted benzene ring; ring C represents an optionally further substituted aromatic ring; R1 represents a lower alkyl optionally substituted by optionally substituted hydroxy; X1a represents a bond or optionally substituted lower alkylene; X1b represents a bond or optionally substituted lower alkylene; X2 represents a bond, O, or S; X3 represents a bond or an optionally substituted divalent hydrocarbon group; and Y represents optionally esterified or amidated carboxy) are prepared A process for preparing I is disclosed. Thus, (2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(3-hydroxy-2,2- dimethylpropyl)-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-yl]methyl]-1,3- thiazol-5-yl)acetic acid was prepared in a multistep process from 2-(tert-butoxycarbonylamino)acetic acid and potassium monoethyl malonate. Compds. of this invention are said to show IC50 values of \leq 1 μM against squalene synthase. Formulations are given. 839723-04-5P 839723-05-6P 839723-06-7P ΙT 839723-07-8P 839723-08-9P 839723-09-0P 839723-10-3P 839723-11-4P 839723-12-5P 839723-13-6P 839723-14-7P 839723-15-8P 839723-16-9P 839723-17-0P 839723-21-6P 839723-22-7P 839723-23-8P 839723-24-9P 839723-26-1P 839723-27-2P 839723-28-3P 839723-30-7P 839723-31-8P 839723-32-9P 839723-33-0P 839723-34-1P 839723-35-2P 839723-36-3P 839723-37-4P 839723-38-5P 839723-39-6P 839723-40-9P 839723-41-0P 839723-43-2P 839723-44-3P 839723-45-4P

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazepine derivs. as squalene synthase inhibitors) ${\rm RN} = 839723 - 04 - 5 \;\; {\rm CAPLUS}$

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-05-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-06-7 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-\text{chloro}-5-(2,3-\text{dimethoxyphenyl})-1,2,3,5-\text{tetrahydro}-1-(3-\text{hydroxy}-2,2-\text{dimethylpropyl})-2-\text{oxo}-4,1-\text{benzoxazepin}-3-yl]methyl]-<math>\alpha$, α -dimethyl- (CA INDEX NAME)

RN 839723-07-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-08-9 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-09-0 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-10-3 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl](CA INDEX NAME)

Absolute stereochemistry.

RN 839723-11-4 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[[1-(hydroxymethyl)cyclobutyl]methyl]-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-12-5 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[[1-(hydroxymethyl)cyclobutyl]methyl]-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-13-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-propyl-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-14-7 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(CA INDEX NAME)

Absolute stereochemistry.

RN 839723-15-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-ethyl-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-16-9 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-

1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-17-0 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-21-6 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy- (CA INDEX NAME)

RN 839723-22-7 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-23-8 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (CA INDEX NAME)

RN 839723-24-9 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-26-1 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-27-2 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- β -hydroxy- (CA INDEX NAME)

RN 839723-28-3 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-thiazolyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-30-7 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, calcium salt (1:1) (CA INDEX NAME)

Ca

RN 839723-31-8 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl-, calcium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Ca

RN 839723-32-9 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-33-0 CAPLUS

CN 5-Oxazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-34-1 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- α , α -dimethyl- (CA INDEX NAME)

RN 839723-35-2 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-ethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-36-3 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(CA INDEX NAME)

Absolute stereochemistry.

RN 839723-37-4 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-38-5 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-propyl-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-39-6 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-ethyl-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-40-9 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-41-0 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-43-2 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 4-carboxy-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-44-3 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 4-carboxy-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-45-4 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 4-carboxy-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-46-5 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 4-carboxy-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-47-6 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(2-carboxyphenyl)-, 4-ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-48-7 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(3-carboxyphenyl)-, 4-ethyl ester (CA INDEX NAME)

RN 839723-49-8 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(4-carboxyphenyl)-, 4-ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-50-1 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-51-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(3-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-52-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(4-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-54-5 CAPLUS

CN 2-Propenoic acid, 3-[1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-1H-pyrazol-5-yl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-57-8 CAPLUS

CN 1,3,4-Oxadiazole-2-acetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-58-9 CAPLUS

CN 1,3,4-Thiadiazole-2-acetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-59-0 CAPLUS
CN 1,3,4-Thiadiazole-2-propanoic acid,
5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-60-3 CAPLUS
CN 1,2,4-Oxadiazole-4(5H)-acetic acid,
3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-61-4 CAPLUS
CN 1,2,4-Oxadiazole-4(5H)-acetic acid,
3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo-(CA INDEX NAME)

Absolute stereochemistry.

RN 839723-62-5 CAPLUS
CN 1,2,4-Oxadiazole-5-propanoic acid,
3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-63-6 CAPLUS

CN 1,2,4-Oxadiazole-5-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-65-8 CAPLUS

CN 1H-1,2,4-Triazole-5-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839723-66-9 CAPLUS

CN Benzoic acid, 3-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-67-0 CAPLUS

CN Benzoic acid, 3-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-68-1 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 839723-69-2 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-70-5 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-ethoxy-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 839723-71-6 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-72-7 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 5-(carboxymethoxy)-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-73-8 CAPLUS

CN 2-Propenoic acid, 3-[4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-74-9 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-75-0 CAPLUS

CN 2-Propenoic acid, 3-[4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-76-1 CAPLUS

CN 2-Propenoic acid, 3-[3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839723-77-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839723-78-3 CAPLUS

CN Benzenepropanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

RN 839723-79-4 CAPLUS

CN Benzenepropanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-80-7 CAPLUS

CN Benzenepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-81-8 CAPLUS

CN Benzenebutanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-

3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-82-9 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-83-0 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

RN 839723-86-3 CAPLUS

CN Acetic acid, 2-[4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenoxy]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-87-4 CAPLUS

CN Benzeneacetic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

RN 839723-89-6 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-90-9 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(2-phenylethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-91-0 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(2-phenylethyl)- (CA INDEX NAME)

RN 839723-93-2 CAPLUS

CN 1H-Pyrazole-5-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-94-3 CAPLUS

CN 1H-Pyrazole-4-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

RN 839723-95-4 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-96-5 CAPLUS

CN 1H-Pyrazole-3-propanoic acid, $1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$ -hydroxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-97-6 CAPLUS

CN 1H-Pyrazole-5-propanoic acid, $1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$ -hydroxy- (CA INDEX NAME)

RN 839723-98-7 CAPLUS

CN 2-Propenoic acid, 3-[1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-1H-pyrazol-4-yl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-99-8 CAPLUS

CN

1,3,4-Thiadiazole-2-butanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839724-00-4 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-01-5 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-02-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, calcium salt (2:1) (CA INDEX NAME)

●1/2 Ca

RN 839724-03-7 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethylene)-, (α Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839724-04-8 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -hydroxy-, (α R)- (CA INDEX NAME)

RN 839724-05-9 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$, β -dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-06-0 CAPLUS

CN 5-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

RN 839724-07-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-10-6 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-11-7 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

RN 839724-12-8 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$ -hydroxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-13-9 CAPLUS

CN 2-Propenoic acid, 3-[2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-4-thiazolyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839724-14-0 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-15-1 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$, β -dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-16-2 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

RN 839724-17-3 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-18-4 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (CA INDEX NAME)

RN 839724-19-5 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-20-8 CAPLUS

CN 2-Thiopheneacetic acid, 5-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-22-0 CAPLUS

CN 5-Thiazoleacetic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

RN 839724-23-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-24-2 CAPLUS

CN 4-Thiazoleacetic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

RN 839724-26-4 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-29-7 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl](CA INDEX NAME)

Absolute stereochemistry.

RN 839724-30-0 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (CA INDEX NAME)

RN 839724-32-2 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-(CA INDEX NAME)

Absolute stereochemistry.

RN 839724-33-3 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-34-4 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-

(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-35-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-36-6 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839724-37-7 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-38-8 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_3C$$
 ON
 R
 OMe
 OMe
 OMe

RN 839724-39-9 CAPLUS
CN 1,2,4-Oxadiazole-5-propanoic acid,

3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-40-2 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-41-3 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

RN 839724-42-4 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-43-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- β -methyl-, (β R)- (CA INDEX NAME)

CN Acetic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-45-7 CAPLUS

CN Propanoic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-46-8 CAPLUS

CN Acetic acid, 2-[[1-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]-1-methylethyl]thio]- (CA INDEX NAME)

RN 839724-47-9 CAPLUS

CN Acetic acid, 2-[[1-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]-1-methylethyl]thio]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-48-0 CAPLUS

CN Acetic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]- (CA INDEX NAME)

RN 839724-49-1 CAPLUS

CN Propanoic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-50-4 CAPLUS

CN Acetic acid, 2-[[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-25-6 CAPLUS

CN Propanoic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]-2-methyl- (CA INDEX NAME)

RN 839725-26-7 CAPLUS

CN Butanoic acid, 4-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-27-8 CAPLUS

CN Acetic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (CA INDEX NAME)

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-29-0 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-30-3 CAPLUS
CN 1,2,4-Oxadiazole-5-pentanoic acid,
3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-

Absolute stereochemistry.

(CA INDEX NAME)

RN 839725-31-4 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-32-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

HO2C
$$(CH_2)$$
3 N (CH_2) 3 R S $C1$ MeO OMe

RN 839725-33-6 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-34-7 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-35-8 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (CA INDEX NAME)

RN 839725-36-9 CAPLUS

CN 1,3,4-Oxadiazole-2-butanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-37-0 CAPLUS

CN 1,3,4-Oxadiazole-2-propanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839725-38-1 CAPLUS

CN 5-Thiazolepropanoic acid, $4-[[(3R,5S)-7-\text{chloro}-5-(2,3-\text{dimethoxyphenyl})-1,2,3,5-\text{tetrahydro}-1-(3-\text{hydroxy}-2,2-\text{dimethylpropyl})-2-\text{oxo}-4,1-\text{benzoxazepin}-3-yl]methyl]-<math>\beta$ -hydroxy- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-39-2 CAPLUS

CN 2-Propenoic acid, 3-[4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839725-40-5 CAPLUS

CN 5-Thiazolepropanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839725-41-6 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-42-7 CAPLUS

CN 2-Thiophenebutanoic acid, 5-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

RN 840494-06-6 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (CA INDEX NAME)

Absolute stereochemistry.

```
ΙT
    839724-52-6P 839724-57-1P 839724-60-6P
    839724-62-8P 839724-63-9P 839724-64-0P
    839724-66-2P 839724-67-3P 839724-70-8P
    839724-71-9P 839724-72-0P 839724-73-1P
    839724-74-2P 839724-75-3P 839724-76-4P
    839724-78-6P 839724-79-7P 839724-81-1P
    839724-82-2P 839724-84-4P 839724-85-5P
    839724-86-6P 839724-87-7P 839724-88-8P
    839724-90-2P 839724-91-3P 839724-92-4P
    839724-94-6P 839724-95-7P 839724-96-8P
    839724-97-9P 839724-98-0P 839724-99-1P
    839725-00-7P 839725-04-1P 839725-06-3P
    839725-07-4P 839725-14-3P 839725-17-6P
    839725-43-8P 839725-44-9P 839725-47-2P
    839725-48-3P 839725-49-4P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzoxazepine derivs. as squalene synthase inhibitors) 839724-52-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN

RN 839724-57-1 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-60-6 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-62-8 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -oxo-, ethyl ester (CA INDEX NAME)

RN 839724-63-9 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-64-0 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, ethyl ester, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839724-66-2 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-67-3 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-70-8 CAPLUS

CN 5-Thiazolecarboxylic acid, 4-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-2-methyl-, ethyl ester (CA INDEX NAME)

RN 839724-71-9 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-72-0 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (CA INDEX NAME)

RN 839724-73-1 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-74-2 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-75-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

RN 839724-76-4 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(ethoxycarbonyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-78-6 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-, ethyl ester (CA INDEX NAME)

RN 839724-79-7 CAPLUS

CN 1H-Pyrazole-3-acetic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-81-1 CAPLUS

CN 1,3,4-Oxadiazole-2-acetic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

RN 839724-82-2 CAPLUS

CN 1,3,4-Thiadiazole-2-acetic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-84-4 CAPLUS

CN 1,3,4-Thiadiazole-2-propanoic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-85-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-3-[(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)methyl]-5-(2,3-dimethoxyphenyl)-1,5-dihydro-, (3R,5S)- (CA INDEX NAME)

RN 839724-86-6 CAPLUS

CN 1,2,4-Oxadiazole-4(5H)-acetic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-87-7 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-ethoxy-1H-pyrazol-1-yl]-, ethyl ester (CA INDEX NAME)

RN 839724-88-8 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-90-2 CAPLUS

CN 2-Propenoic acid, 3-[4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, ethyl ester, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839724-91-3 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (CA INDEX NAME)

RN 839724-92-4 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-94-6 CAPLUS

CN Benzeneacetic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (CA INDEX NAME)

RN 839724-95-7 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-96-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-97-9 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)-, ethyl ester (CA INDEX NAME)

RN 839724-98-0 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-99-1 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- α - (hydroxyphenylmethyl)-, ethyl ester (CA INDEX NAME)

RN 839725-00-7 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- α -(phenylmethylene)-, ethyl ester, (α Z)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839725-04-1 CAPLUS

CN 4-Thiazolepropanenitrile, $2-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-<math>\alpha$ -[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-06-3 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxypheny1)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropy1)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]-, ethyl ester (CA INDEX NAME)

RN 839725-07-4 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-14-3 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-17-6 CAPLUS

CN Acetic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-

1,2,4-thiadiazol-5-yl]thio]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-43-8 CAPLUS

CN Propanoic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]-2-methyl-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-44-9 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-47-2 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]-1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-, ethyl ester (CA INDEX NAME)

RN 839725-48-3 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-49-4 CAPLUS

CN 1,3,4-Oxadiazole-2-propanoic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
```

AN 2003:767796 CAPLUS Full-text

DN 139:276921

TI Preparation of benzoxazepine derivatives as squalene synthetic enzyme inhibitors

IN Miki, Takashi; Kori, Masaki

PA Takeda Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 36 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 2

	PATENT NO.									APPLICATION NO.					DATE			
ΡΙ	JP CA	2003277377 2513170			A 20031002				CA 2	2004-		20040115						
	WO	2004064865			A1		2004	20040805			2004-	JP23		20040115				
		W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BΖ,	CA,	CH,
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			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	KΖ,	LC,
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						,		RO,	,									
	JP 2004107361			A 20040408					JP 2	2004-		20040116						
	JP 2004315500			A 20041111					JP 2	2004-		20040116						
	US 20060052362				A1 20060309				US 2	2005-		20050713						
	US	US 20080113965 A1 2				2008	20080515 US 2008-6506							20080103				
PRAI	JP 2002-10623			A 20020			0118											
	JΡ	2003	-101	25		А		20030117										
	JΡ	2003	-935 ¹	91		Α		2003	0331									
	WO	2004	-JP2	34		W		2004	0115									
	US	2005	-542	322		A1		2005	0713									
OS GI																		

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [wherein W = halo; R1 = alkyl; R2 = CHO or (un)substituted alkyl; m = 1-3; n = 0-2; R4 = H or -(CH2)p-R5; R5 = (un)substituted CO2H; p = 0-3; etc.] and salts and prodrugs thereof are prepared as squalene synthetic enzyme inhibitors. I are useful as a lipid decrease medicine and a high fat blood disease medicine (no data). Thus, the compound II was prepared in a multi-step synthesis. II showed IC50 of 45 nM against human squalene synthetic enzyme. Formulations containing I as an active ingredient were also described.

IT 606928-79-4P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-79-4 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

Absolute stereochemistry.

IT 606928-80-7P 606928-81-8P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-80-7 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 606928-81-8 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 606928-73-8P 606928-75-0P 606928-77-2P 606928-78-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-73-8 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,6-tetrahydro-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-75-0 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-3-[2-(3,4-dihydro-1(2H)-pyridinyl)-2-oxoethyl]-5-(2,3-dimethoxyphenyl)-1,5-dihydro-, (3R,5S)- (CA INDEX NAME)

RN 606928-77-2 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethyl-3-oxopropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-78-3 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, methyl ester (CA INDEX NAME)

IT 606928-74-9P 606929-11-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-74-9 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,6-tetrahydro- (CA INDEX NAME)

Absolute stereochemistry.

RN 606929-11-7 CAPLUS

CN 4-Pyridineacetic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro- (CA INDEX NAME)

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L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN AN 2003:22711 CAPLUS \underline{\text{Full-text}}
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DN 138:83384

- TI Preventives/remedies for organ functional disorders with increasing ubiquinone and inhibiting squalene synthase
- IN Sugiyama, Yasuo; Nishimoto, Tomoyuki; Kiyota, Yoshihiro
- PA Takeda Chemical Industries, Ltd., Japan
- SO PCT Int. Appl., 121 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese

FAN.CNT 1

r An.	PATENT NO.					KIN	D	DATE		APPLICATION NO.						DATE			
ΡI	WO	7O 2003002147			A1	_	20030109			WO 2	 002-	20020627							
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KR,	KΖ,	LC,	LK,	LR,	LS,	
			LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	PL,	
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	
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								CM,											
	CA 2451163 AU 2002313277								CA 2002-2451163										
									AU 2002-313277							0020			
	JΡ	JP 2003081873							JP 2002-188133						2	0020	627		
	EΡ	1407																	
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			•	,	•	,	,	RO,	,	,	,								
	US 20040204500							US 2003-480707											
		2006								US 2006-473560									
		2008				A1				US 2008-9277						20080117			
PRAI		2001				А		2001											
		2002				W		2002											
		2003				_		2003											
		2006				В1		2006	0623										
OS	MAF	RPAT	138:	8338	4														

- AB Preventives/remedies for organ functional disorders, preventives/remedies for organ dysfunction and preventives/remedies for obesity and sequels thereof which contain a compound having an effect of increasing ubiquinone, its salt or prodrugs of the same; and ubiquinone increasing agents containing a compound having a squalene synthase inhibitory effect, its salt or prodrugs of the same.
- IT 189060-33-1 189060-48-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Preventives/remedies for organ functional disorders with increasing ubiquinone and inhibiting squalene synthase)

RN 189060-33-1 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-5-ylmethyl)-, (3R,5S)- (CA INDEX NAME)

RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-5-ylmethyl)-, (3R,5S)-(CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5
        ANSWER 9 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
ΑN
        2002:368342 CAPLUS Full-text
DN
        136:359669
        High-density lipoprotein-cholesterol level elevating agent
ΤI
        Nishimoto, Tomoyuki; Tozawa, Ryuichi; Kori, Masakuni; Amano, Yuichiro
IN
        Takeda Chemical Industries, Ltd., Japan
PA
SO
        PCT Int. Appl., 111 pp.
        CODEN: PIXXD2
DT
        Patent
LA
        Japanese
FAN.CNT 1
        PATENT NO.
                                         KIND
                                                       DATE
                                                                    APPLICATION NO.
                                           ____
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                                           A1 20020516 WO 2001-JP9802
        WO 2002038180
                                                                                                                   20011109
PΤ
               W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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        CA 2428669
                                            A1
                                                     20020516
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        AU 2002012741
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                                                                                                                     20011109
                                            Α
                                                       20020521
        JP 2002205956
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                                                                                                                     20011109
                                                       20080827
        JP 4138299
                                            В2
                                                  20030806 EP 2001-981043
                                           A1
        EP 1332763
                                                                                                                     20011109
               R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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        US 20040063750
                                           A1
                                                     20040401
                                                                           US 2003-416239
                                                                                                                     20030506
        US 20080058310
                                            A1
                                                      20080306
                                                                            US 2007-810887
                                                                                                                     20070607
PRAI JP 2000-342607
                                            Α
                                                      20001109
        WO 2001-JP9802
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                                                     20011109
        US 2003-416239
                                          A1 20030506
        MARPAT 136:359669
OS
         Disclosed is a novel high-d. lipoprotein (HDL)-cholesterol level elevating
AΒ
         agent containing a compound which has a squalene synthase inhibitory effect.
         The HDL-cholesterol-elevating effect of N-[[(3R,5S)-1-(3-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy
         dimethylpropyl)-7-chloro-5-(2,3- dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-
         4,1-benzoxazepine-3- yl]acetyl]piperidine-4-acetic acid (I) in common marmoset
         was examined Also, a tablet containing I 50, D-mannitol 50, corn starch 33.9,
         croscarmellose sodium 40, hydroxypropyl cellulose 5.5, and magnesium stearate
         0.6 mg was prepared
TΤ
        189060-33-1 189060-48-8
        RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
              (high-d. lipoprotein-cholesterol level elevating agents containing squalene
              synthase inhibitors)
RN
        189060-33-1 CAPLUS
CN
        4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-
        methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-
        5-ylmethyl)-, (3R,5S)- (CA INDEX NAME)
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RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-5-ylmethyl)-, (3R,5S)-(CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5
    ANSWER 10 OF 10 CAPLUS COPYRIGHT 2009 ACS on STN
AN 1997:317788 CAPLUS <u>Full-text</u>
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DN 126:293368

OREF 126:56816h,56817a

TI Benzoxazepine compounds, their production and use as lipid lowering agents

Yukimasa, Hidefumi; Sugiyama, Yasuo; Tozawa, Ryuichi ΙN

PA Takeda Chemical Industries, Ltd., Japan

SO PCT Int. Appl., 112 pp.

CODEN: PIXXD2

DT Patent

LA English																				
F'AN.	CNT 1 PATENT NO.										APPLICATION NO.									
ΡI	WO 9710224									WO 1996-JP2596							9960:	912		
		W:	AL,	AM,	AU,	AZ,			BG,									GE,	HU,	
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		2231							1113		CA	13	790-	2231	052		1	9900.	914	
		9669									ΑIJ	10	996-	6944	2		1	9960:	912	
		0913								AU 1996-69442 JP 1996-242378										
		3479							1215											
	EP	8625								EP		1996-930		9303	0365				912	
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GI	₹,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	FI		_														
		1196	052			A C			1014		CN	19	996-	1968	92		1	9960	912	
		1072 1097	049			A1		2001			EP 2000-126672					10000010				
		1097				B1		2001			EP 2000-126672					19960912				
	EL								FR,	GB.	GF	₹.	TT.	T.T.	T.U.	NI	SE.	MC.	PT.	
		- · ·	IE,		011,	22,	<i>D1</i> (,	,	,	02,	0.	,	,	,	,	112,	22,	110,	/	
	AT	2027				Τ		2001	0715		ΑT	19	996-	9303	65		1	9960	912	
	ES	2158	344			Т3		2001	0901					9303			1	9960	912	
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	US 6613761 JP 2001097963			B1		2003														
		4021		63		A B2		2001 2007			JP 2000-323310					20001018				
		3036				T3		2007			GR 2001-401564					20010926				
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		2007				A1			0524					6380						
		2007				A			1227					2105			2	0061: 0070:	810	
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PRAI	JP	1995	-235	457		А		1995	0913											
		1996				А3		1996												
		1996				А3		1996												
		1996				W		1996												
		1997				A		1997												
		1998				A3		1998												
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		2000				B1		2000												
		2005				B1		2005												
OS		RPAT			68	-		_000												

New benzoxazepines I [R = alkyl, hydroxyalkyl; R1 = alkyl; R2 = halogen; R3 = (un)substituted CONH2, heterocyclic group having a deprotonatable hydrogen atom]were prepared for use as cholesterol and triglyceride lowering agent. Thus, I [R = CH2CMe3, R1 = Me, R2 = C1, R3 = CO2H] was amidated, dehydrated to the nitrile, and cyclized with Me3SiN3 to give I [R = CH2CMe3, R1 = Me, R2 = C1, R3 = 5-tetrazolyl] which had a squalene synthetase inhibiting IC50 of 11X10-9 M.

IT 189060-33-1P 189060-48-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylbenzoxazepinones as hypolipemic agents)

RN 189060-33-1 CAPLUS

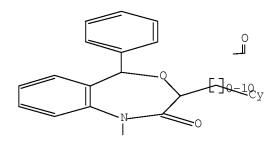
CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-5-ylmethyl)-, (3R,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2H-tetrazol-5-ylmethyl)-, (3R,5S)-(CA INDEX NAME)

=> d 12; d his; log y
L2 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 20:09:13 ON 28 FEB 2009)

FILE 'REGISTRY' ENTERED AT 20:09:44 ON 28 FEB 2009

L1 STRUCTURE UPLOADED

L2 QUE L1 L3 14 S L2

L4 211 S L2 FUL

FILE 'CAPLUS' ENTERED AT 20:10:22 ON 28 FEB 2009

L5 10 S L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	57.40	243.50
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-8.20	-8.20

STN INTERNATIONAL LOGOFF AT 20:11:47 ON 28 FEB 2009